

Day 3 overview

- Making scripts
- Understanding compute clusters
- Using Slurm with SBATCH scripts
- Troubleshooting SBATCH scripts
- Transferring and downloading files

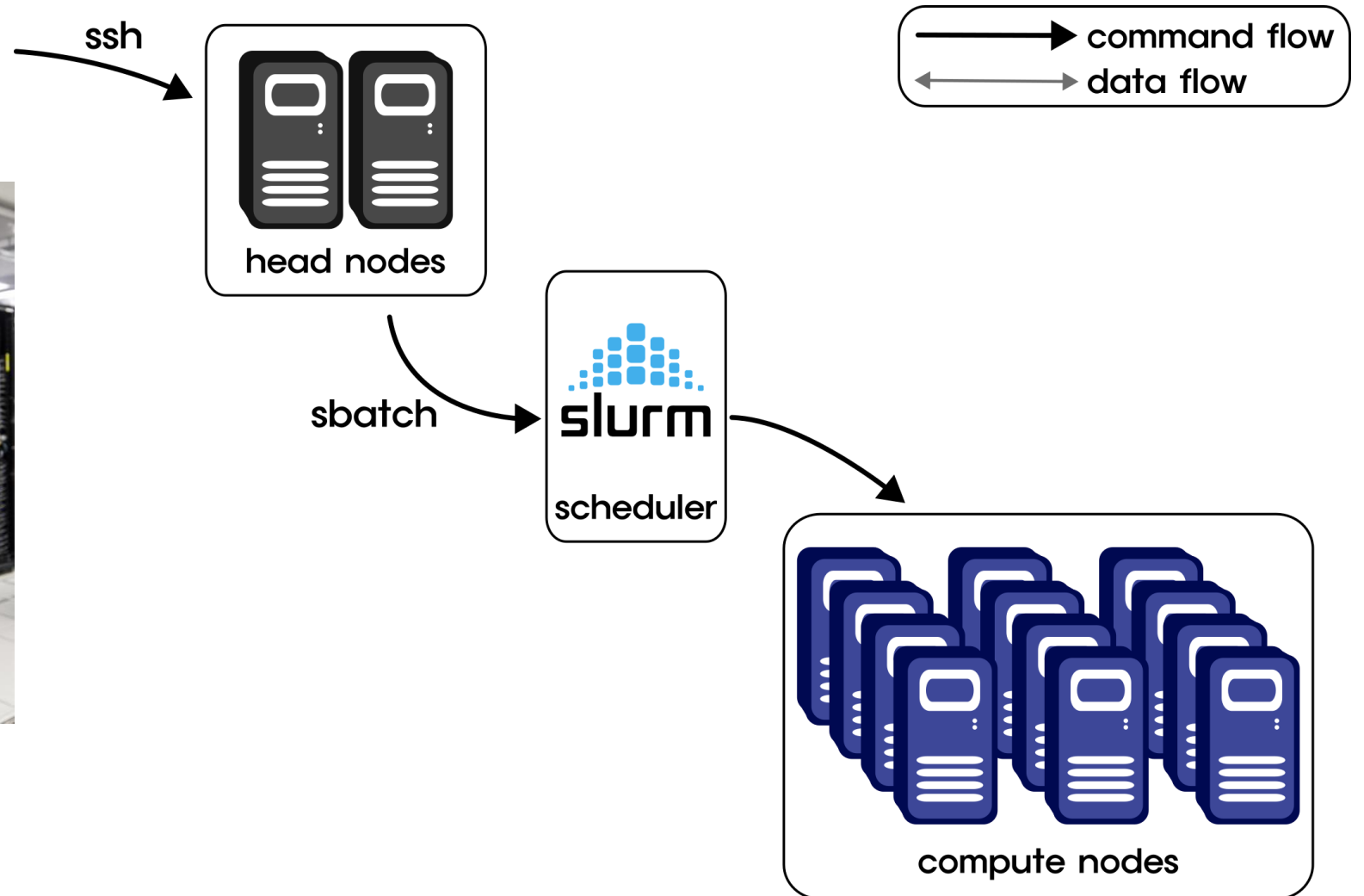
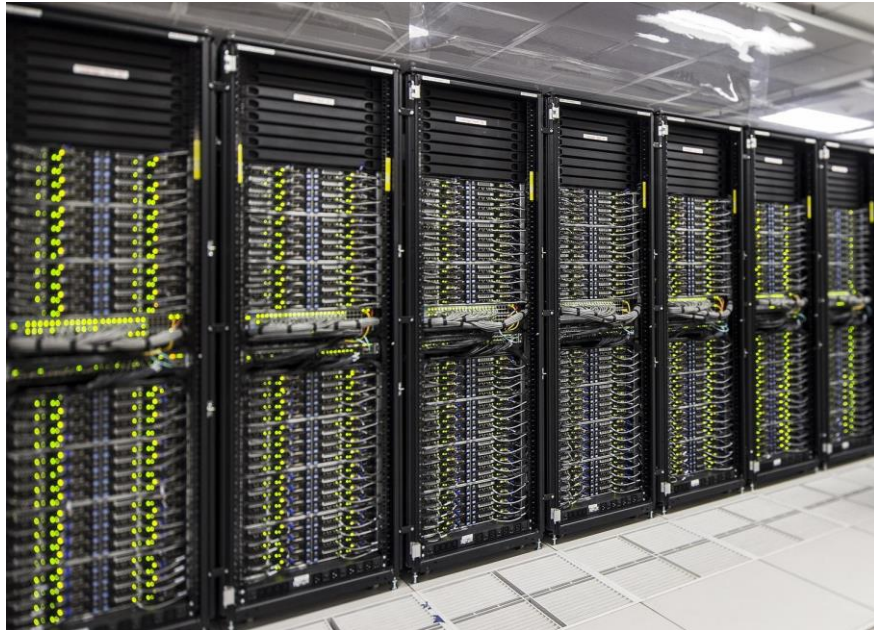
Make a script

- In a terminal on your local machine:
 - Open a new file called `test_script.sh`
 - Add the following four lines:

```
#!/bin/bash  
pwd  
sleep 3  
echo "This is a test script"
```
 - Save and exit, then run the script with:

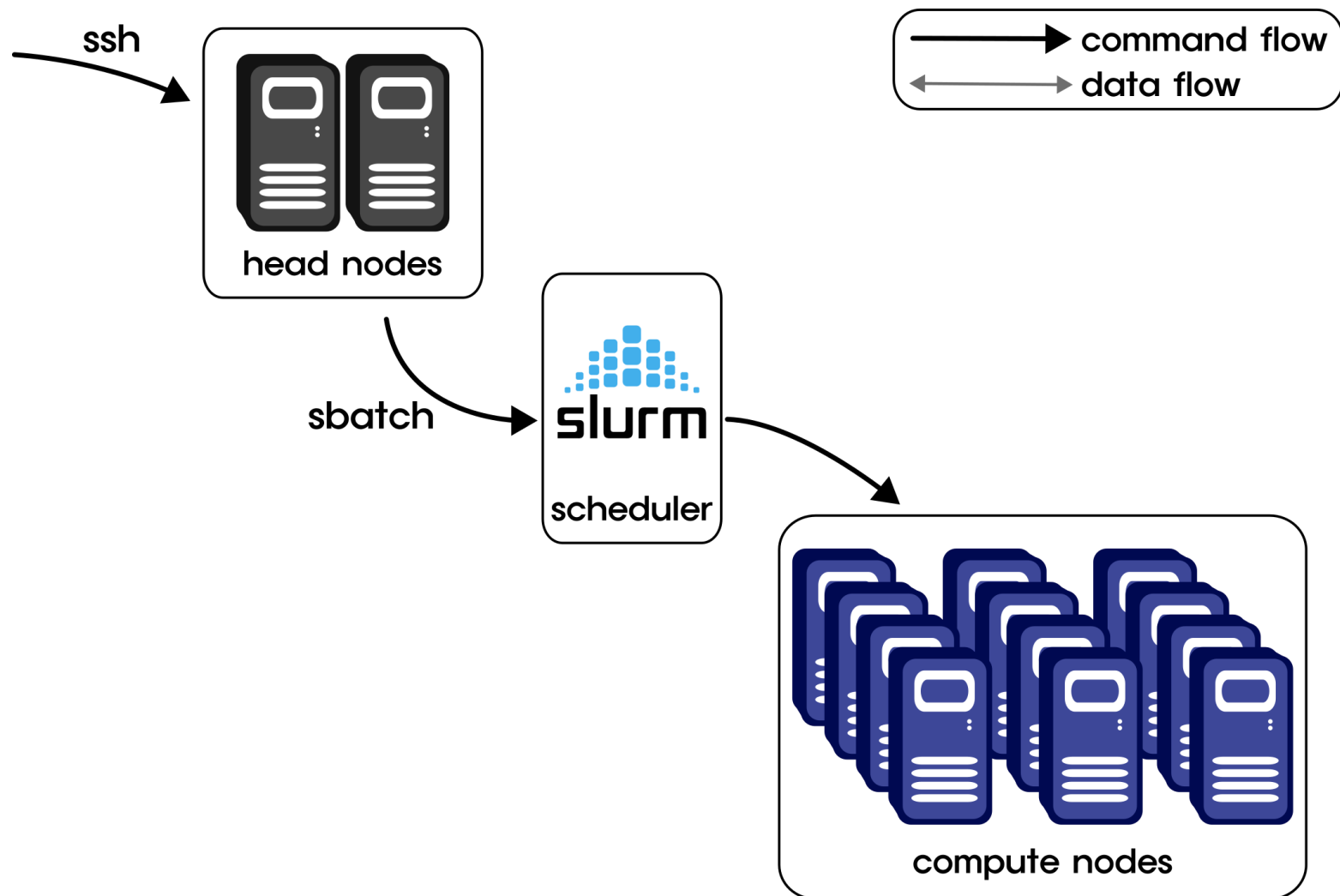
```
sh test_script.sh
```

Compute cluster architecture



Compute cluster architecture

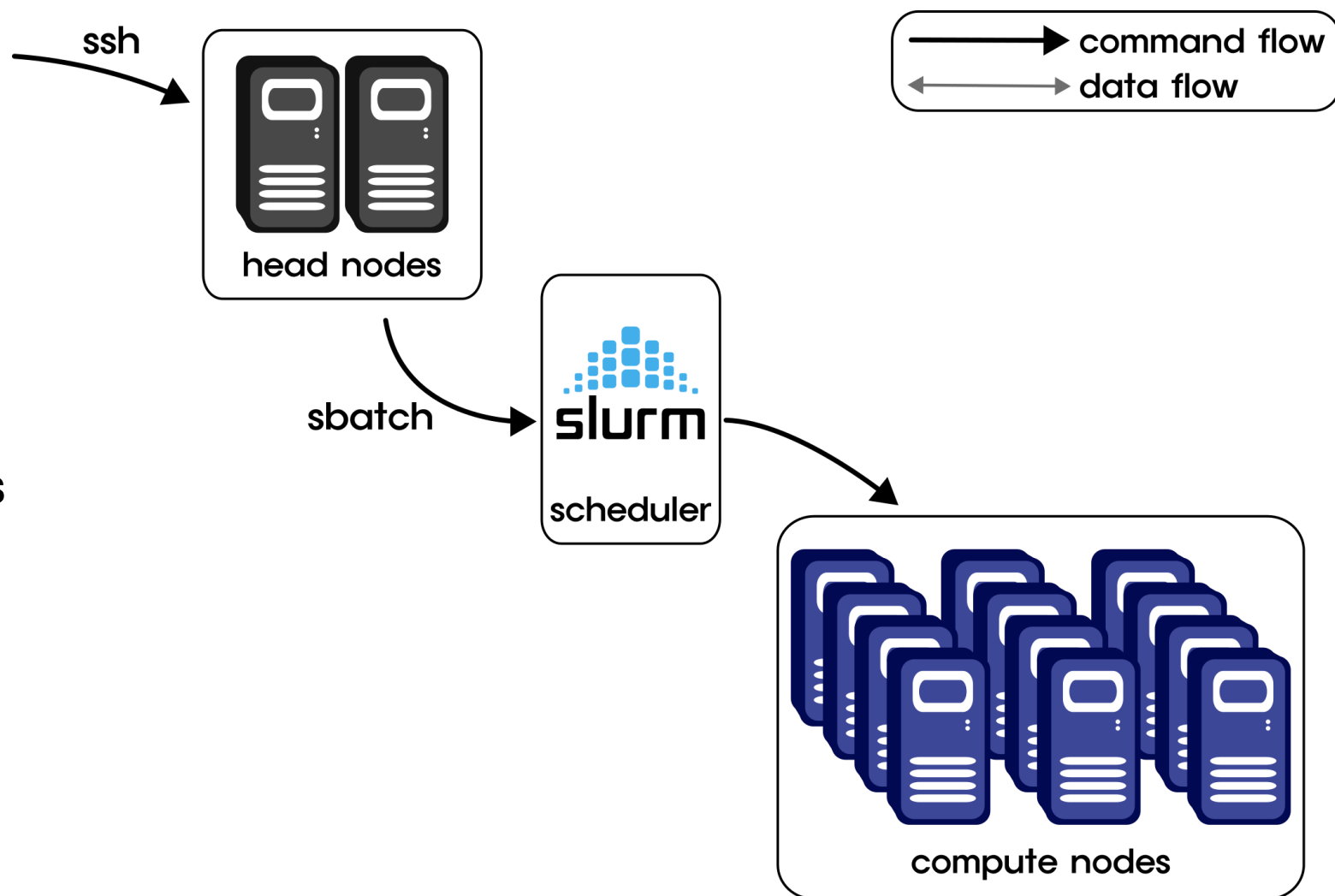
- Head nodes
 - Very limited resources
 - Only intended for basic interfacing/commands
- Compute nodes
 - Extensive resources
 - Take job scripts (lists of commands)
 - Require a scheduler to manage resources



Compute cluster architecture

- Slurm (scheduler)

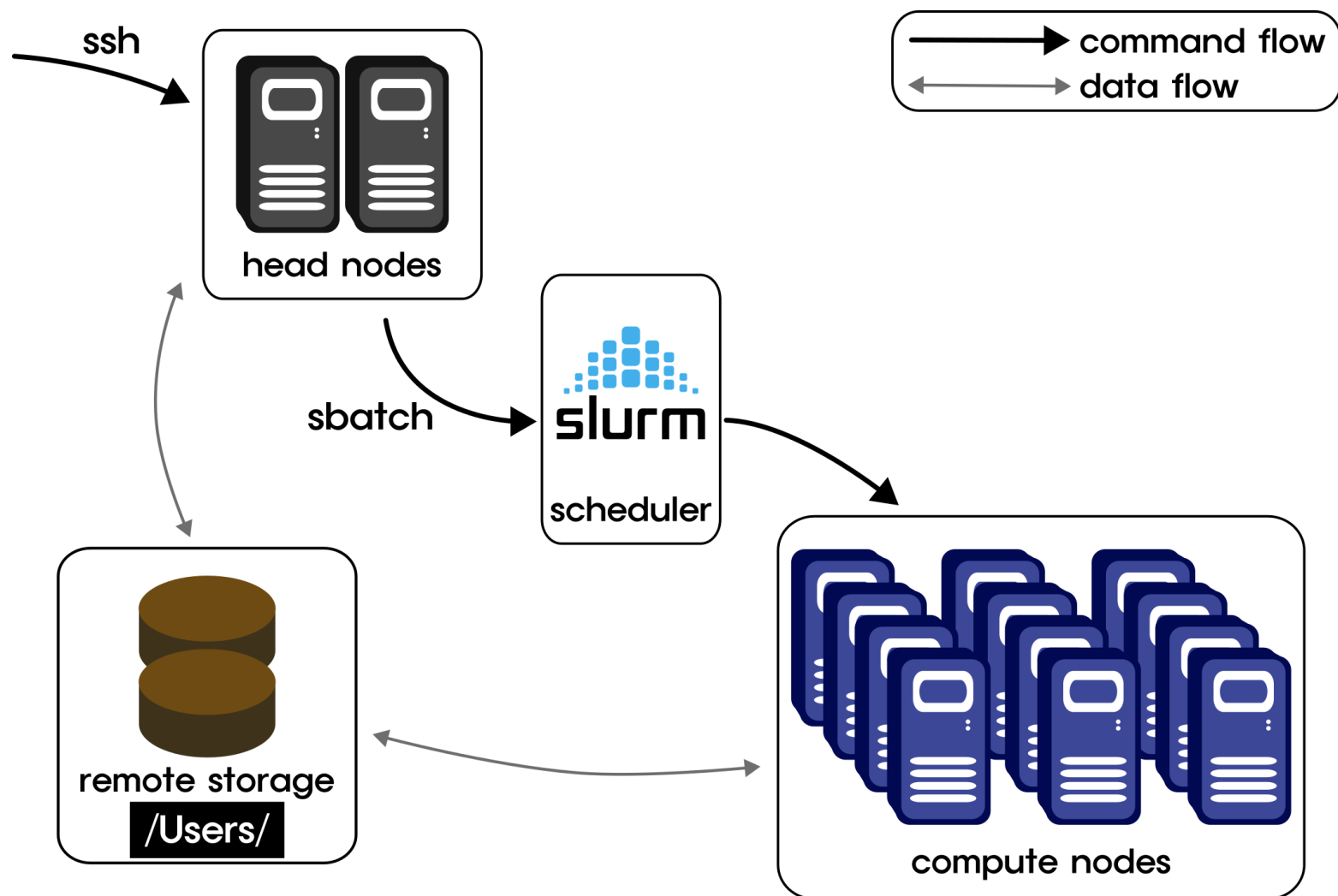
- Manages resources to execute jobs
- Executes jobs as resources become available



Compute cluster architecture

- Remote storage

- Off-site from cluster (slow)
- Backed up
- For Fiji, located under `/Users/<username>`



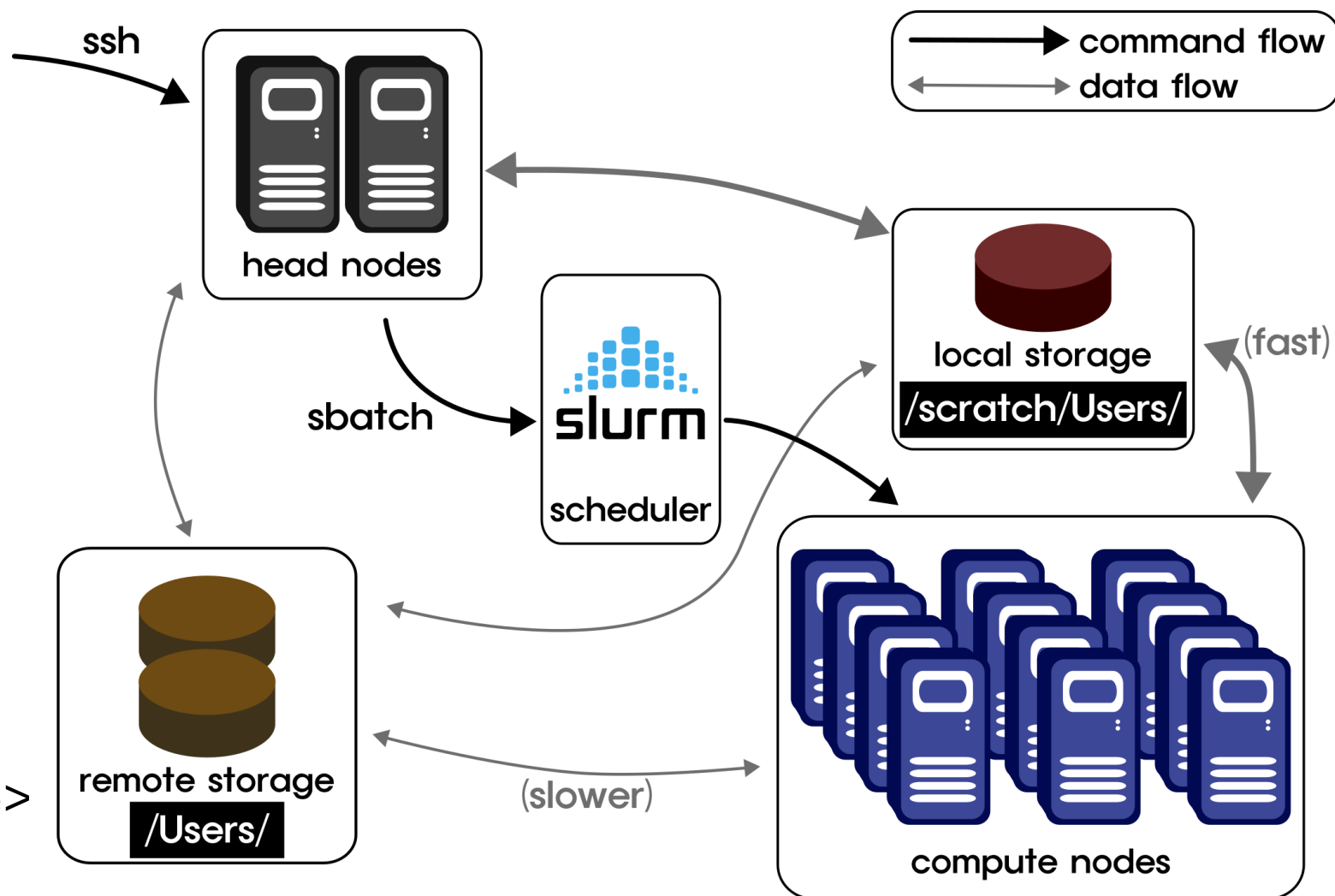
Compute cluster architecture

- Remote storage

- Off-site from cluster (slow)
- Backed up
- For Fiji, located under `/Users/<username>`

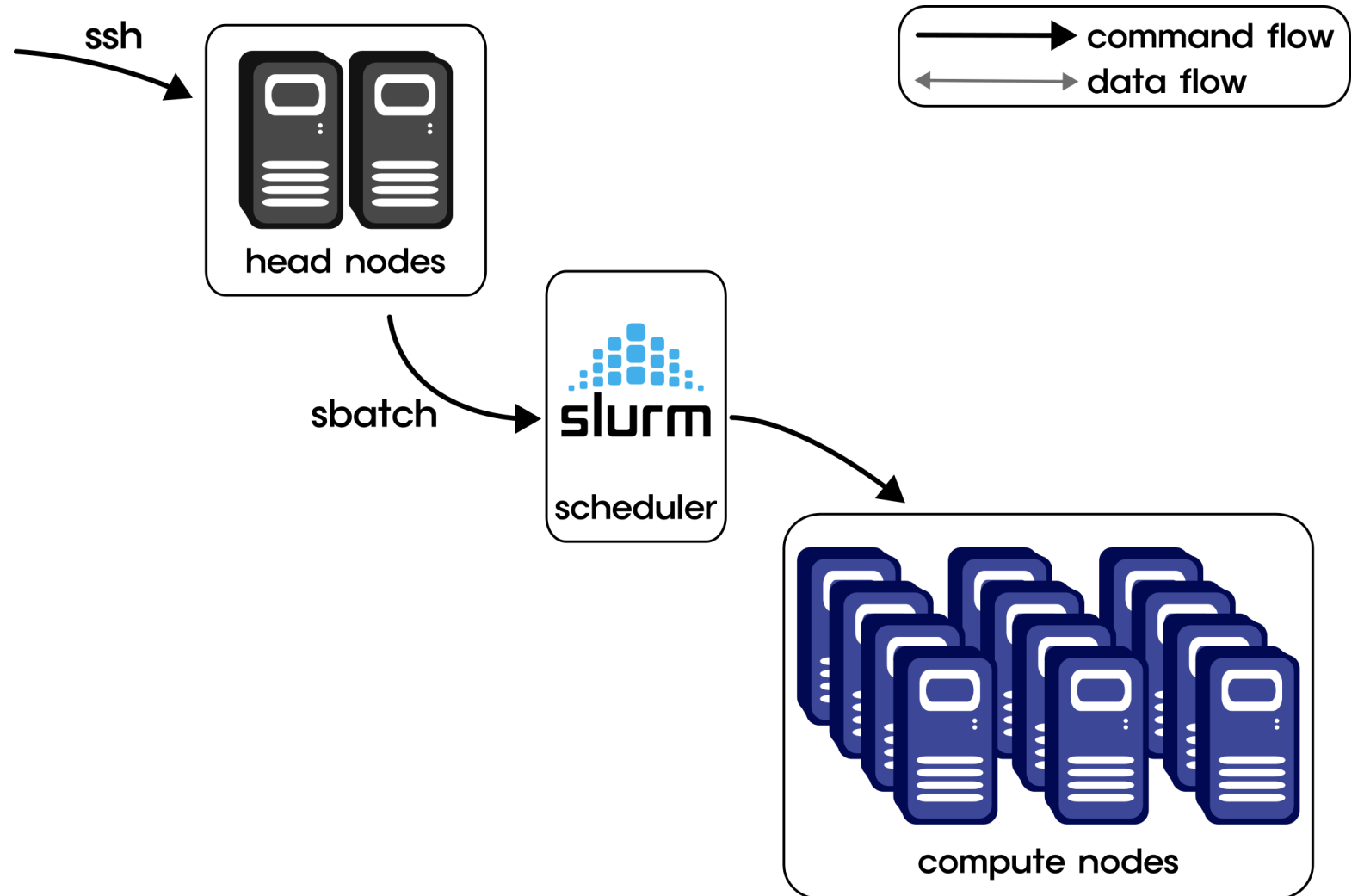
- Local storage

- On-site with cluster (fast)
- NOT backed up, \$\$\$
- For Fiji, located under `/scratch/Users/<username>`



Run a job!

- Day 3 worksheet Part 1
 - Create an SBATCH script with a header and a command
 - Run the script as a job
 - Troubleshoot



SBATCH header

```
#!/bin/bash
```

```
#SBATCH -p <partition> → specify job partition (queue) to run the job
```

```
#SBATCH --time=00:00:00 → hrs:minutes:seconds
```

```
#SBATCH --mem=<memory>
```

```
#SBATCH --ntasks= → how many cores/processors are needed for the job
```

```
#SBATCH --job-name=<jobname> → give the job a name
```

```
#SBATCH --mail-type=ALL
```

```
#SBATCH --mail-user=<you@email.com>
```

```
#SBATCH --error=<path>/%x_%j.err → specify name and location of error file
```

```
#SBATCH --output=<path>/%x_%j.out → specify name and location of log file
```

Output/error files are primarily used for troubleshooting:

- These files capture STDERR and STDOUT that isn't captured within the script
- %x and %j are Slurm variables that will be **automatically** filled into the filenames
- %x is the job name. If not specified in the header, it will be the name of your sbatch script file
- %j is the unique job ID assigned to your job by Slurm
- Using these variables ensures that you'll always have unique filenames for every job

- How to know when a job fails
 - Expected files are empty or missing
 - Job finishes much quicker than expected
 - Errors appear in your error file
- Why does a job fail?
 - Incorrect command/parameters
 - Incorrect paths
 - Incorrect SBATCH header
 - Incorrect file format
 - Issues with software versions



BREAK

Understanding Modules

- Environmental variables alter how we interact with the cluster or help us “find” commands
 - An important environmental variable is `$PATH`, which specifies where the computer looks for commands
(look at it with `echo $PATH`)
- Modules are set up by admin and allow you to easily change environmental variables
 - Not present on every compute cluster
 - Modules are automatically unloaded after a session terminates

Module commands

<code>module avail</code>	List available modules
<code>module spider</code>	Describe modules (with tab complete)
<code>module load <module></code>	Load specific module
<code>module list</code>	List currently loaded modules
<code>module unload <module></code>	Unload specific module
<code>module purge</code>	Unload all current modules

Analyze data!

- Day 3 worksheet Part 2
 - In your SBATCH script, write a command to run the program FastQC
 - Run the script as a job
 - Troubleshoot if necessary
 - Transfer the HTML output to your local computer and view it

Homework for day 4

- Videos for day 3 (if not already done)
- Videos for day 4
- Homework_day3.md worksheet